

An Evaluation of Ground State Energy of Two Dimensional Liquid ^4He at Various Densities

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ABSTRACT

Using theoretical formulation of Chung-In Um et al., the ground state energy of two-dimensional liquid ^4He interacting through Lenard-Jones and Aziz potential were calculated at various densities. Our theoretical result indicates that ground state energy of two dimensional liquid ^4He interacting with Aziz potential is close to GFMC calculation.

Keywords: Lenard –Jones potential, Aziz potential, GFMC Calculation, Ground State Energy, Two –dimensional liquid ^4He .

1. INTRODUCTION

For many years, physicist have used hyper netted (HNC) and Fermi hyper netted chain (FHNC) theories to investigate the properties of highly correlated interacting boson and fermion systems such as liquid ^4He and normal liquid ^3He ^{1,2}. The HNC/FHNC equations with Jastrow ground-state wave functions treat consistently both long and short correlations of the system and give agreements to some degree with experimental results. In spite of qualitative successes of the Jastrow ground-state

function, there exist quantitative differences between HNC/FHNC results and experimental ones, especially the equilibrium ground-state energy, and this fact leads one to consider the contributions arising from the three-body correlation functions.³ It is well known that the three-body correlations do not affect seriously the structural properties of ground states, such as the radial distribution function and liquid structure function, but contribute significantly to the ground-state energy. Since liquid ^3He system is less dense than liquid ^4He , that is, the equilibrium density of

the former is 0.0166 \AA^{-1} while that of the latter is 0.02185 \AA^{-3} in a three-dimensional system, effects of three-body correlations in ^3He are rather small compared to those in ^4He . At equilibrium density, they make up about half the difference between the Jastrow results and experimental energy in a liquid ^3He system⁵ and lower the Jastrow ground-state energy by about 10 % in liquid ^3He .

A trial ground-state wave function including three-body correlation functions in addition to two-body correlation effects can be constructed in the form

$$\psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{i < j} f_2(r_{ij}) \prod_{i < j < k} f_3(r_{ij}, r_{jk}, r_{ki}) |\Phi\rangle = F|\Phi\rangle$$

Where $f_2(r_{ij})$ is the two-body correlation function which describes spatial correlations and depends only upon the spatial distance r_{ij} between two particle $f_3(r_{ij}, r_{jk}, r_{ki})$ is a three-body correlation function, and $|\Phi\rangle$ is the anti-symmetric product of non-interacting single-particle plane waves normalized in the system's area Ω with N fermions, which becomes simply unity for boson systems.

In addition to the three-body correlation functions in the ground-state wave function, one should take into account the contributions coming from the elementary diagrams as well as effects of the HNC/FHNC equations to obtain better results. Unfortunately, there does not exist a general closed expression for the elementary diagrams and therefore one must calculate each diagram individually, which is very time consuming. During the last two decades, two approximations for the estimation of the elementary diagrams have

been developed. One is known as the scaling approximation⁴ and the other is the interpolating equation approximation⁵. Both techniques have shown their efficiency for central two-body correlations, providing similar results for the total ground-state energy to those of the variational Monte Carlo simulation. The scaling approximation uses the fact that successive contributions of the five, six and higher order elementary diagrams are approximately proportional to and have very similar spatial behaviour to the body elementary diagrams,⁴ so that one can represent the total elementary diagram contribution by means of the readily calculable four-body elementary diagrams. The interpolating equation approximation determines a parameter such that it gives the same value for the classical isothermal compressibility obtained from both the HNC/FHNC equations and Percus-Yevick⁶ equations using the classical pressure derivative or the compressibility integral.

Although large number of theoretical works regarding ^4He and ^3He system have been reported⁷⁻¹¹ but very few of them have been used for two-dimensional liquid.

Chung-In Um *et al.*¹² have developed a theoretical model to study two-dimensional quantum fluid. By taking their model, one has evaluated the radial distribution function $g(r)$ as a function of r for two dimensional liquid ^4He interacting through Aziz potential for various densities. In section 2, we have given the mathematical formulae used in the evaluation. The discussion of the result has been given in section 3 of this paper. In the last portion, we have shown the tables of the results and the reference taken.

2. MATHEMATICAL FORMULAE USED IN THE EVALUATION

The Hamiltonian for the considered system is given by

$$H = T + V = \sum_i T_i + \sum_{i < j} V_{ij} = -\frac{\hbar^2}{m} \sum_i \nabla_i^2 + \sum_{i < j} V(|\vec{r}_i - \vec{r}_j|) \quad (1)$$

Where $V(r)$ is the interatomic interaction. A popular potential theoretical investigations is that of Lenard-Jones, which has parameters, i.e., the hard-core radius and

the well depth, and can be written as

$$V_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], \epsilon = 1022 K, \sigma = 2.556 \text{ \AA} \quad (2)$$

However, $V_{LJ}(r)$ includes only the dipole-dipole interaction and does not take into account multiple interactions. A more physically realistic potential which accounts for the self-consistent field Hartree-Fock repulsion and multiple interactions is the HFDHE² potential of Aziz *et al.*¹³ presented as

$$V_{LJ}(r) = \epsilon^* \left[A \exp\left(-\alpha \frac{r}{r_m}\right) - \left\{ c_6 \left(\frac{r_m}{r} \right)^6 + c_8 \left(\frac{r_m}{r} \right)^8 + c_{10} \left(\frac{r_m}{r} \right)^{10} F(r) \right\} \right] \quad (3)$$

Where

$$F(r) = \begin{cases} \exp[-(Dr_m/r - 1)^2] & r/r_m \leq D \\ 1 & r/r_m > D \end{cases} \quad (4)$$

The values of the constants are

$$\begin{aligned} A &= 0.54485 \times 10^6, & \epsilon^*/k_B &= 10.8 \\ \alpha &= 13.353384, & C_6 &= 1.3732412 \\ C_8 &= 0.4253785, & C_{10} &= 0.178100 \\ D &= 1.241314, & r_m &= 2.9673 \text{ \AA} \end{aligned}$$

It is well known from the Green's function Monte Carlo simulations and other variational calculations that the Aziz potential gives closer results to experiments than V_{LJ} in three dimensions. One uses both potentials and compare the results with those in two dimensions.

The n-particle distribution function is represented as

$$P_n(\vec{r}_1, \dots, \vec{r}_n) = v^n N(N-1) \times \frac{\int \psi^+(\vec{r}_1, \dots, \vec{r}_n) \psi(\vec{r}_1, \dots, \vec{r}_n) d\vec{r}_{n+1} \dots d\vec{r}_N}{\langle \psi | \psi \rangle} \quad (5)$$

Where \vec{r}_i denotes the spatial coordinates of the i^{th} particle and v is the spin degeneracy of the system (2 for this system). In homogeneous system, as $N \rightarrow \infty$

and $\Omega \rightarrow \infty$, the single-particle distribution function reduces to the density of the system so that the radial distribution function can be expressed in terms of the density and two-particle distribution function $P_2(r)$ as

$$g(r) = \frac{1}{\rho^2} p_2(r) = N(N-1) \left(\frac{v}{\rho} \right)^2 \frac{\int \psi^+(\vec{r}_1, \dots, \vec{r}_n) \psi(\vec{r}_1, \dots, \vec{r}_n) d\vec{r}_3, \dots, d\vec{r}_N}{\langle \psi | \psi \rangle} \quad (6)$$

One uses the FHNC approximation to sum the diagrams arising from the cluster properties of $g(r)$. In this scheme, $g(r)$ can be decomposed as

$$g(r_{ij}) = g_{dd}(r_{ij}) + 2g_{de}(r_{ij}) + g_{ee}(r_{ij}) \quad (7)$$

Where dd, de and ee represent terms in which both i and j are not exchanged, only j is exchanged, and both i and j are exchanged, respectively. The components of $g(r_{ij})$ are given by

$$\begin{aligned} g_{dd}(r_{ij}) &= \exp[u_2(r_{ij}) + N_{dd}(r_{ij}) + E_{dd}(r_{ij})] \\ g_{de}(r_{ij}) &= g_{dd}(r_{ij}) [N_{de}(r_{ij}) + E_{de}(r_{ij})] \\ g_{ee}(r_{ij}) &= g_{dd}(r_{ij}) [-L^2(r_{ij}) / v + N_{ee}(r_{ij}) \\ &\quad + E_{ee}(r_{ij}) + (N_{ee}(r_{ij}) + E_{ed}(r_{ij}))^2] \\ g_{ee}(r_{ij}) &= g_{dd}(r_{ij}) L(r_{ij}) / v \end{aligned} \quad (8)$$

where

$$L(r_{ij}) = -l(k_F r_{ij}) + v(N_{ee}(r_{ij}) + E_{ee}(r_{ij})) \quad (9)$$

$$l(x) = 2j_1(x) / x \quad (10)$$

k_F is the Fermi momentum of the system, and $j_1(x)$ is the Bessel's function of the first kind of order 1. N_{mm} represent sums of the diagrams and E_{nm} sums of the elementary diagrams. The equation $g_{ee}(r_{ij})$ denotes the terms in which both i and j are exchanged in incomplete exchange loop, and $N_{ee}(r_{ij})$ and $E_{ee}(r_{ij})$ are sums of the nodal diagrams and the elementary diagrams in which i and j belong to the same permutation loop, respectively.

With the FHNC equation and expression for the $g(r)$, one now calculates the energy per particle of the system

$$\frac{E_{\text{var}}}{N} = \frac{1}{N} \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\langle V \rangle}{N} + \frac{\langle T \rangle}{N} \quad (11)$$

The potential energy per particle is expressed by taking the thermodynamic limit, i.e., the area of system Ω and the number of particles N are infinite, keeping the density constant as

$$\frac{\langle V \rangle}{N} = \frac{\rho}{2} \int d\vec{r}_{ij} V(r_{ij}) g(r_{ij}) \quad (12)$$

The expression for the kinetic energy part is more complicated. There are three well-known expressions for the helium system i.e., Jackson-Feenberg¹⁴, Clark-Westhous¹⁵ and Bethe-Pandharipande¹⁶. Among expressions for the kinetic energy per particle the Jackson-Feenberg form is popular and easily tractable since its three-particle distribution part is not more significant than others. One uses here the Jackson-Feenberg and the Bethe-Pandharipande forms so that we make use of the scaling approximation for the elementary diagrams. From the identity

$$\int \psi^\dagger \nabla^2 \psi d\vec{r} = \frac{1}{4} \int [\psi^\dagger (\nabla^2 \psi) (\nabla^2 \psi^\dagger) + -2(\nabla \psi^\dagger) \cdot (\nabla \psi) d\vec{r}] \quad (13)$$

Jackson-Feenberg energy form is obtained as

$$\begin{aligned}
 \frac{E_{JF}}{N} &= \frac{-\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \left\langle \Phi \left| F^2 \nabla^2 \nabla_i^2 + \frac{1}{2} F \nabla_i^2 F - \frac{1}{2} (\nabla_i F)^2 \right| \Phi \right\rangle \\
 &\quad + \frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i F^2 \nabla_i^2 |\Phi|^2 d\vec{r}_1 \dots d\vec{r}_N + \frac{\langle V \rangle}{N} \\
 &= T_F = W_B + W_\phi + U_\phi
 \end{aligned} \tag{14}$$

The first term of Eq. (13), $T_F = \hbar^2 k_F^2 / 4m$, is the non interacting fermion energy with the Fermi momentum $k_F = [4\pi\rho/v]^{1/2}$, and the second, W_B is the energy of the boson system.

$$W_B = \frac{\rho}{2} \int d^2 r g(r) \left[V(r) - \frac{\hbar^2}{(2m)} \frac{\nabla^2 f_2(r) - (\nabla f_2(r))^2}{f_2(r)} \right] \tag{15}$$

The forms of W_ϕ and U_ϕ are

$$\begin{aligned}
 W_\phi &= \frac{\hbar^2 \rho}{4mv} \int d^2 r \{ g_{dd}(r) - 1 [1(k_F r) - v(N_{ee}(r) + E_{ee}(r))] \\
 &\quad \times \nabla^2 1(k_F r) + \nabla 1(k_F r)^2 - v d_{dd}(r) E_{ee}(r) \nabla^2 1(k_F r) \}
 \end{aligned} \tag{16}$$

$$\begin{aligned}
 U_\phi &= \frac{\hbar^2 \rho^2}{8m} \int d^2 r_1 d^2 r_2 d^2 r_3 (g_{dd}(r_{12}) - 1) \nabla 1(k_F r_{12}) \cdot (g_{dd}(r_{13}) - 1) \\
 &\quad \times \nabla 1(k_F r_{13}) g_{ee}(r_{23})
 \end{aligned} \tag{17}$$

$$U_\tau = \frac{\hbar^2 \rho}{16m} \int d^2 r_1 d^2 r_2 d^2 r_3 g_3(r_{12}, r_{23}, r_{13}) \nabla^2 u_3(r_{12}, r_{23}, r_{13}) \tag{18}$$

Pandharipande-Bethe energy form is obtained by expanding the kinetic energy per particle as

$$-\frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \left\langle \Phi \left| F \nabla_i^2 [F | \Phi] \right. \right\rangle = \frac{\langle T \rangle_{PB}}{N} \tag{19}$$

From which one gets,

$$\frac{\langle T \rangle_{PB}}{N} = -\frac{\hbar^2}{2mN} \frac{1}{\langle \psi | \psi \rangle} \sum_i \left\langle \Phi \left| F [\nabla_i^2 + \nabla_i^2 + 2(\nabla_i F)] \right| \Phi \right\rangle \tag{20}$$

After some calculations, we obtained E_{PB}/N as

$$\frac{E_{PB}}{N} = T_F + W + W_F + U + U_F \tag{21}$$

Where W and U are the bosonic energies per particle, and W_F and U_F are from the last term of Eq. (19)

$$W = \frac{\rho}{2} \int d^2 r g(r) \left[V(r) - \left(\frac{\hbar^2}{m} \right) \frac{\nabla^2 f_2(r)^2}{f_2(r)} \right] \tag{22}$$

$$U = -\frac{\hbar^2 \rho^2}{2m} \int d^2 r_1 d^2 r_2 d^2 r_3 g_3(r_{12}, r_{23}, r_{13}) \left[\frac{\nabla_1 f_2(r_{12}) \cdot \nabla_1 f_2(r_{13})}{f_2(r_{12}) f_2(r_{13})} \right] \tag{23}$$

$$W_F = -\frac{\hbar^2 \rho}{2m} \int d^2 r g_{ee}(r) \left[\frac{\nabla f_2(r) \cdot \nabla 1(k_F r)}{f_2(r)} \right] \tag{24}$$

$$\begin{aligned}
 U_F &= -\frac{\hbar^2 \rho^2}{2m} \int d^2 r_1 d^2 r_2 d^2 r_3 \nabla f_2(r_{12}) \cdot \nabla 1(k_F r_{13}) \\
 &\quad \times \{ g_{ee}(r_{13}) g_{dy}(r_{12}) (g_{dy}(r_{32}) - 1) + g_{dd}(r_{13}) g_{ee}(r_{23}) g_{ee}(r_{31}) \}
 \end{aligned} \tag{25}$$

For numerical calculations, one adopts the McMillan type function as a trial two-body correlation function, which is widely used in variational and Monte Carlo calculations for liquid and helium systems.

$$u_2(r) = -\left(\frac{b}{r}\right)^5 \quad (26)$$

Where, b is a variational parameter chosen to give an optimized distribution function at a given density. To obtain more precise results, we include three-body correlation effects in the following forms:

$$u_3(r_{ij}, r_{jk}, r_{ki}) = \sum_{eye} \eta(r_{ij}) \eta(r_{jk}) (\hat{r}_{ij} \cdot \hat{r}_{jk}) \quad (27)$$

$$\eta(r) = \sqrt{\lambda_1 r} \exp \left[-\left(\frac{r - r_1}{\omega_1} \right)^2 \right] \quad (28)$$

Where cyc denotes the cyclic permutation among the three particles coordinates i, j and k , and i is a unit vector along the line connecting particle i and j . Since it was first used in a variational Monte Carlo calculation,⁸ this form for the three-body correlations is generally used in variational HNC/FHN methods.¹⁻³

Table T₁

Evaluated results of ground state energy of two-dimensional liquid ⁴He interacting through the Lenard-Jones potential at various density

$\rho(\text{\AA}^{-2})$	Ground state energy $E(k)/N$		
	Our cal. results	Chang's ¹⁷ results	GFMC Calculations ⁸
0.020	-0.520	-0.628	-0.504
0.025	-0.546	-0.637	-0.546
0.030	-0.624	-0.658	-0.589
0.035	-0.658	-0.586	-0.627
0.040	-0.748	-0.552	-0.553
0.045	-0.786	-0.505	-0.524
0.050	-0.842	-0.486	-0.508
0.055	-0.725	-0.453	-0.493
0.060	-0.556	-0.446	-0.486

Table T₂

Evaluated results of ground state energy $E(k)/N$ of two-dimensional liquid ^4He interacting through Aziz potential at various densities

$\rho(\text{\AA}^{-2})$	Ground state energy $E(k)/N$		
	Our cal. results	Chang's ¹⁷ results	GFMC Calculations ⁸
0.020	-0.487	-0.586	-0.523
0.025	-0.509	-0.603	-0.588
0.030	-0.586	-0.658	-0.602
0.035	-0.627	-0.709	-0.657
0.040	-0.723	-0.682	-0.597
0.045	-0.706	-0.596	-0.602
0.050	-0.658	-0.542	-0.524
0.055	-0.532	-0.506	-0.486
0.060	-0.456	-0.487	-0.442

3. DISCUSSION OF RESULTS

In this paper, we have evaluated the ground state energy of two dimensional liquid ^4He interacting through Lenard-Jones and Aziz potential at various densities. We have used the theoretical formalism of Chung-In Um *et al.*¹² in our evaluation. Chung-In Um¹² calculated ground state energy of two dimensional liquid ^4He using Jastrow two body correlation function in the trial wave function within the HNC approximation. His other calculation for energy per particle is by taking two body correlation and contribution of order

elementary diagrams. We have taken three body as well as two -body correlations within the scaling approximation.⁴ Our theoretically evaluated results of ground state energy $E(k)/N$ are shown in table T1 and T2 for Lenard –Jones potential and Aziz potential for various densities. We have compared our theoretical results with Chang's result¹⁷ and GFMC result⁸ Our theoretical calculation indicates that the two dimensional liquid ^4He interacting through Aziz potential is more close to the calculation.⁸ Comparing with two potential, one conclude that Aziz potential is more suitable to describe, the ground state of the

two dimensional helium system similar to bulk case¹⁸. Some recent¹⁹⁻²¹ results reveal the same fact.

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